Computational Fluid Dynamics
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Lecture No. # 28
Part 1: Combination of Iteration & Elimination Techniques
Part 2: Introduction to Gradient Search Methods

Till now, what we have done? We have seen some iterative methods and some elimination methods; what we have seen also some of the merits and demerits of this methods; and possibly, what is interesting to see is that is it a viable option that we combine the elimination method with the iteration methods. And that is indeed possible, let us consider an example or a particular method which does it, that is called as line by line TDMA.

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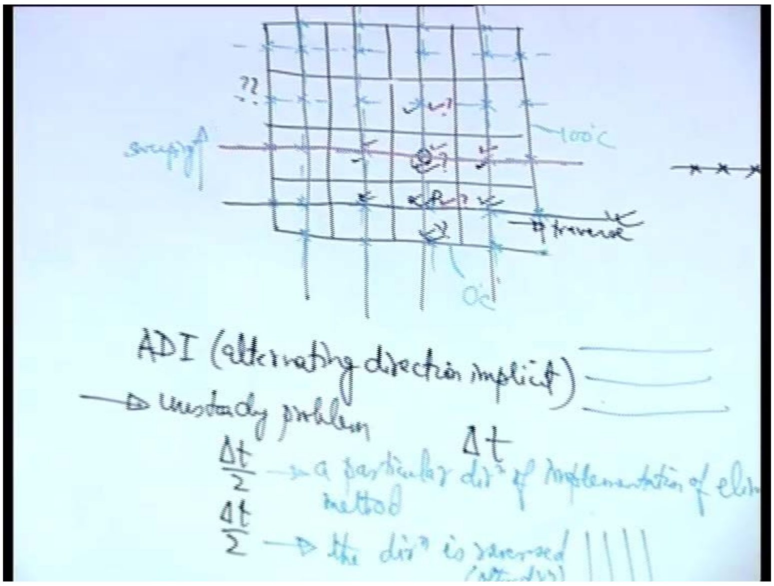

So, we have earlier seen that the TDMA is a very efficient elimination method, and it has the computational complexity of the order of n; at the same time the problem or rather than the limitation with the TDMA is that you cannot use it directly for problems, which have the corresponding coefficient matrices with more number of diagonals than three, like if you have a two-dimensional discretization with five diagonals involved in such cases that the if you have a pentadiagonal matrix, then you cannot directly use the TDMA.

So, why it is so? If you consider a domain…

Usually in finite volume method, what we do? If we have the control volumes, then we consider grid lines like this, which run midway between the control volumes, and this the points where these grid lines intersects, these are the grid points plus you also included grid points at the boundary, to incorporate the boundary conditions these points are also located on the grid lines. You have seen that very purposefully the grid layout is such that corner points are avoided; because corner points are points of singularity so to say, if you for example, take an instance, where let us say that it is a heat transfer problem, these boundary at a temperature of 100 degree centigrade, these boundary at a temperature of 0 degree centigrade. The question comes that what is the temperature of this corner? Can it simultaneously be 0 degree at 100 centigrade? It cannot be physically like that so, this are certain interesting situations, I mean these are the weak points in the analysis, and we always try to avoid this weak points, and to avoid the ambiguity you see that you do not have any grid point really actually lying on this one.

So, you will consider this grid point to be at 0 degree centigrade, these grid point to be at 100 degree centigrade, these point these is not a grid point, these point what? We do not know, god knows. So I mean this can be a big dilemma that if you see this is where there is a weakness in the problem formulation, this is not a weak formulation; this is actually a weak formulation in literal English. So, if you see that, when you have a particular temperature specified at this boundary and particular temperature specified at this boundary, what will be the temperature at this point? Think about it, it is not a straight forward answer; if you say that way it will be 0 plus 100 by 2 or something like that, that is just (( )) statement, I mean it has no scientific basis, but at least during the formulation we have no problem, because this is not included as the part of the gridding system.

Now, let us see that how we intend to solve this problem as a solution of system linear algebraic equation prospective. If you consider any grid point it has four neighbors interior grid point will have four neighbors, boundary will have less number of neighbor. So, the grid point plus the four neighbors will fall five elements of five diagonals the grid point will contribute to the main diagonal and the other points to the immediate next diagonals adjacent to the main diagonal. So, it is a penta diagonal system still let us says, you want to use the TDMA, so you have to then convert the pentadiagonal system into a tri diagonal system; so, tri diagonal system could be there if it was a one dimensional layout with grid points like this; that means, in this example multi dimensionality is bringing the deviation from the tri diagonal system so, what you can do? You can take it as a pseudo tri diagonal system, how? Let us consider this particular grid line.

When we consider this particular grid line, with traverse along this grid line and if we are interested to solve for let us say these grid point then let us identify that, what are its neighbors? It has these four neighbors so the double ticks are the representative of the neighbors of this point p, out of this if you consider the horizontal line the three are there in the same horizontal line, but two are there this one and this one, these are there away from the horizontal line.

So, if some how you would have known the values of the variable at these two point then it would have been a pseudo tri diagonal system, if you would have known these values. Now, how do you know that? You do not, because you do not have the solution. What best you can have? You can have a gauss value or the most recent solution from an iterative scheme. So, if you make an initial guess for the all the grid points and you start with the solution of this line then you take the neighbor values these double tick ones with the question marks these are the neighbors away from the horizontal line, you take these values as the values from the recent iteration.

So, then you are unknowns boil down to three for each grid points and it reduces to a pseudo tri diagonal system. So, then you solve for the TDMA along this horizontal line, once it is done you go to the next horizontal line these line. In the next horizontal line now, if you consider this grid point which we have already marked it has its neighbors four neighbors, I am just taking one example grid point for each horizontal line, but there could be several such grid points just one example we are taking for each horizontal line. So, when you take this horizontal line.

If you have again these three grid points located on the same horizontal line and these two located offset from that, out of that the upper one you can take from the previous iteration and the lower one you can also take from the previous iteration which has been solved immediately before this one so the most current one you can take now the upper one not the most current one, because that line has not yet been solved o that you can take the previous iteration value the lower one you can take the current iteration value so, then you can solve for the TDMA along the next horizontal line. So, you have traversed. So, what you are basically doing, you are having two mechanisms; one is the traversing mechanism you are traversing along each horizontal line and then another is a sweeping mechanism; that is you are sweeping one horizontal line after the other so you are sweeping the horizontal line in the particular direction.

So, in this way, what you are basically doing, the remember that what is the physical essence of solving a CFD problem? A physical essence is how quickly you can make your boundary condition propagate in terms of their effect within the domain o you have a boundary condition here since 0 degree centigrade so in each step this effect is propagated by this distance into the domain in this way once it is wholly swept then it this effect our to the other end. So, if you can make this effect traverse quickly there are certain cases where the effect needs to be traversed quickly to achieve a fast convergence and that can be done in several ways we will come to that, but what we can recognize here is that; the first thing that we are applying the TDMA one line after the other then once we are considering TDMA along a line then all the neighbors which fall for those corresponding lines, the corresponding values are taken as the most recent iterates. So, these are the essential features or essential points so apply TDMA along chosen lines during this, take values of the other neighbors as a recent iterates.

So, what you can see that in this way the boundary condition effect of the boundary condition is propagating from one boundary to inside the domain, but the left boundary also has some boundary condition, and in this way the boundary condition is propagating from bottom to top, but what happens from left to right or left to other direction. So, what you can do is? You can alternate this sweep and traverse direction. So, for example, for one set we have considered that you are taking horizontal line for TDMA then in the next set of iteration you consider the vertical lines, as the lines on which you apply the TDMA and sweep along this direction so you alternate the sweep and traverse direction so that effect of all the boundaries may be propagate inside the domain in an effective way.

So, we can see that, these example is a combination of iteration and elimination so you have essentially and iterative environment where you consider initially guesses for each point, but then when you are solving along lines then along each lines you are applying TDMA which is an elimination method; so, it is a combination of elimination and iteration method. Now, these types of switching direction is many times used in CFD in different method there is a method called as ADI method (alternating direction implicit) the idea of this is straight forward the objective is again like if you alternate the direction of your solution, like your use of the TDMA or the elimination method then you allow the condition at all the boundaries to propagate in an equally effected manner to inside of the domain.

Rather than having a bias towards certain boundary with which is not the case that you want, there are certain cases where a bias to one boundary is what is intended? Like if you have a domain like this where these three boundaries are insulated and these boundaries subjected to a particular temperature say T start at time equal to 0, so it is the effect of the change of the temperature at this boundary that should propagate inside the domain so you can have these as the sweep direction, but this is a special case rather than a general case in a general case you will have effect at all the boundaries equally important, if not unequal.

So, then you expected it to be alternately directed in terms of the sweep and the traverse or you design it to be like that; so that in the most general case also you have the effect of all the boundaries propagating efficiently inside the domain, in the alternating direction implicit method the same principle is used so what is done are you having the total in it, so this is used for an unsteady problem, in an unsteady problem you have the total time interval as delta t each time interval total delta t. So, here what is done is this delta t is divided into 2 parts; delta t by 2 and delta t by 2 so the elimination method is applied over delta t by 2, first delta t by 2 in one direction and in the next delta t by 2 over another direction. So, the basic principle, so the direction of implementation of the elimination method is alternated in every half time interval, because it is alternate, that is why? It is called as alternating direction implicit so you can use a fully time implicit scheme, but in that you have a delta t by 2 and delta t by 2 as half of the time interval so, in this you have a particular direction of implementation of elimination method and here the direction is reversed? Yes; that means, if this was along x direction this would along y direction.

So, if you implement it along x, so if you have horizontal lines along which you solve for the elimination method then in the next case you reverse it so you make it reverse means like the other direction; so, if this is x direction this will be y direction like that. So, we have seen some examples of elimination methods, some examples of iteration method and some examples where we have combinations of elimination and iteration methods, now there are certain method which are neither elimination methods nor iteration methods, but some methods which are fundamentally based on optimization technique and those methods are known as gradient search based methods.

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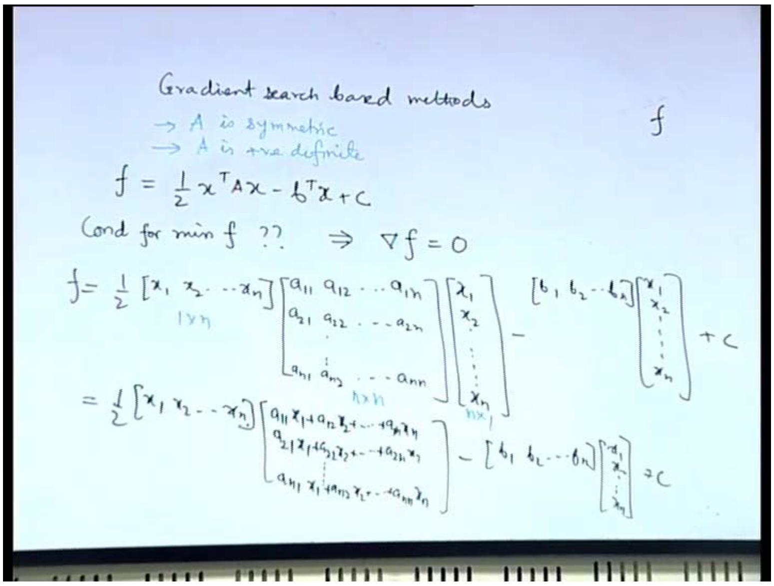

So, we will now get into the gradient search based methods so this method, what it tries to do is? If you have a function f, you know that the gradient of the function represents the maximum rate of change of the function. So, it tries to search a solution of a system of equation by moving into a gradient of a function and how it does to understand that let us consider an example, let us say that we have a function f our objective is to solve the equation system of equation A x equal to b. So, f is equal to half x transpose A x minus b transpose x plus c, where c is an arbitrary constant.

There are two very important restrictions that are imposed; one is A is symmetric and the other is A is positive definite so you can use this method only with this restriction, the next objective is to find out the condition for minimum of f; so, minimum of f implies that the gradient of f must be 0. Let us write in an expanded way, what is f? So, half x transpose x transpose will have x 1, x2 in this way up to x n, a 11 a 1 2 in this ways a 1 n, a 2 1 a 2 2 in this way a 2 n, a n 1 a n 2 in this a n n, this is half x transpose A x minus b transpose b 1 b 2 in this way b n into x plus c.

What is the gradient of f? del f del x 1 del f del x 2 in this way del f del x n so let us find out first, what is del f del x 1 to do that may be let us doing one more step to simplify f. So, let us check the dimensionalities of the system for matrix multiplication compatibility this is n by n this is n by 1 and this is 1 by n so the final result is just a scalar 1 by 1. So, let us write this x 1, x 2 up to x n then multiplication of these two; so, first row with first column a 11 x 1 plus a 1 2 x 2 in this way a 1 n x n, then second row with first column a 2 1 x 1 plus a 2 2 x 2 in this way plus a 2 n x n in this way the last one is a n 1 x 1 plus a n 2 x 2 plus a n n x n you can expand one more step if you want?

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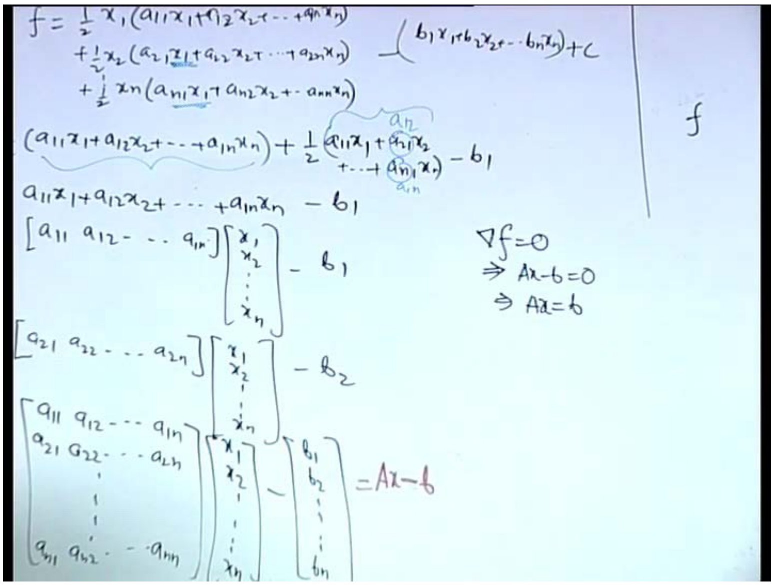

So, f is equal to half x 1 into a 11 x 1 plus a 1 2 x 2 in this way plus a 1 n x n plus half x 2 a 2 1 x 1 plus a 2 2 x 2 this way plus a 2 n x n, in this way plus half x n a n 1 x 1 plus a n 2 x 2 plus a n n x n minus b 1 x 1 plus b 2 x 2 in this way b n x n plus c.

So, what is del f del x 1 So far the first term you use the product rule so it is half into a 11 x 1 plus a 1 2 x 2 plus in this way a 1 n x n then plus half x 1 into the derivative of this term a 1 1 so half a 11 x 1 from the next term, what will come out you have x 1 has this is the term only which has x 1, so the corresponding derivative is half a 2 1 x 2 so a 11 x 1 plus a 2 1 x 2 in this way plus a n 1 x n that is this term minus b 1, c is the constant. Now, because A is symmetric A equal to a transpose; that means, a 1 2 is equal to a 2 1, a n 1 is equal to a 1 n, so in place of a 2 1 it is a 1 2 in place of a 1 n like that. So, then the term in this bracket and the term in this bracket they become the same, so it becomes a 11 x 1 plus a 1 2 x 2 plus in this way a 1 n x n minus b 1 so you can write this as a 11 a 1 2 in this way a 1 n into x 1 x 2 x n minus b 1 similarly, what will be del f del x 2 here in place of a 11 it is a 2 1 a 2 2 in this way a 2 n into x 1 x 2 up to x n minus b 2 so if you write, what is gradient of f that is del f del x 1 del f del x2 in this way del f del x n.

So that you can assemble all these rows, so that finally you will get a1 1 a 1 2 in this way a 1 n for the first row, a 2 1 a 2 2 in this way a 2 n for the second row finally a n 1 a n 2 in this way a n n for the n-eth row. So the first row is for del f del x 1 second row is for del f del x2 in this way row is for del f del x n you can see that, in symbolic form this is nothing but equal to A x minus b. So, setting grade f is equal to 0 is as good as setting A x minus b equal to 0 or getting the corresponding solution as the solution of the system A x is equal to b so in other words we can say that getting g a solution of A x equal to b is as good as extremizing the function f when we say extremizing the function, if we have said the condition grade f equal to 0 it could either be maxima or could be a minimum. In the next stage what we say that, what we do here is indeed a minimization of f, but not maximization how do we show that what we are doing indeed corresponds to the minimum of f, but not a maximum of f that is the next thing that we would see.

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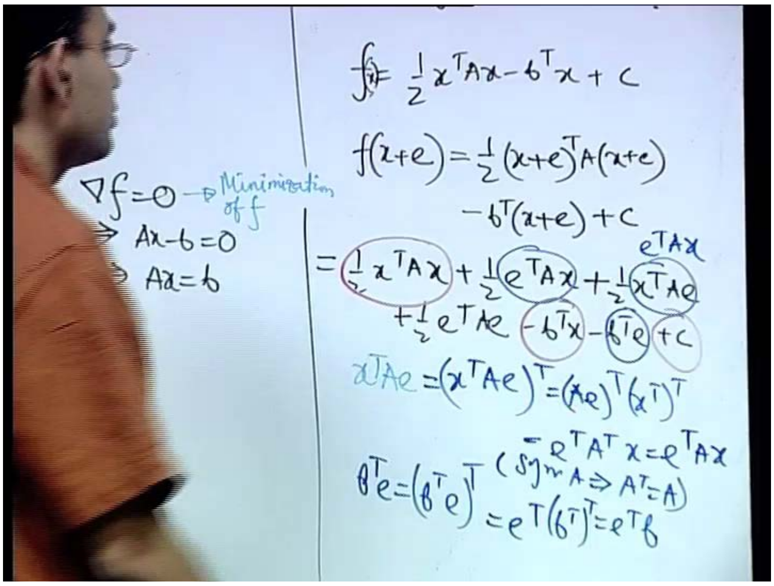

So the next question that would like to answer is why minimization and not maximization so far that let us again write, what is f, half half of x transpose A x minus b transpose x plus c. Let us consider a vector e and find out, what is f (x plus e) if we can show that this is f (x), if we can show that f (x) is the minimum of all possible arguments corresponding to this one that is f (x) is less than f (x plus e) all e; that mean that f (x) is a minimum. So let us write, what is f (x plus e) this is half of x plus e transpose A x plus e remember e is any arbitrary vector minus b transpose x plus e plus c so let is expand these this is the half x transpose A x plus half e transpose A x plus half x transpose A e plus half of e transpose A e minus b transpose x minus b transpose e plus c, from this we can isolate certain terms.

We can isolate half x transpose A x minus b transpose x plus c, because this is f (x). Next we can make certain simplification remember e transpose A x is a scalar so it is just like x transpose A x in place of x it is e, similarly x transpose A e. So, you can write x transpose A e as follows. So, this is same as x transpose A e transpose transpose of a scalar is the scalar itself then you can use a into b transpose equal to b transpose into a transpose so this will be A e transpose into x transpose transpose so this is equal to e transpose A transpose x, because it is because A is symmetric A transpose is equal to A; so, this is e transpose A x because you have symmetric A, this implies A transpose equal to A. So, this term becomes e transpose A x this term has so this is half e transpose A x this term another half e transpose A x, so total together it becomes e transpose A x, then let us consider this b transpose e b transpose e is b transpose e transpose because these also a scalar; so this is equals to e transpose b transpose transpose, so e transposes b.

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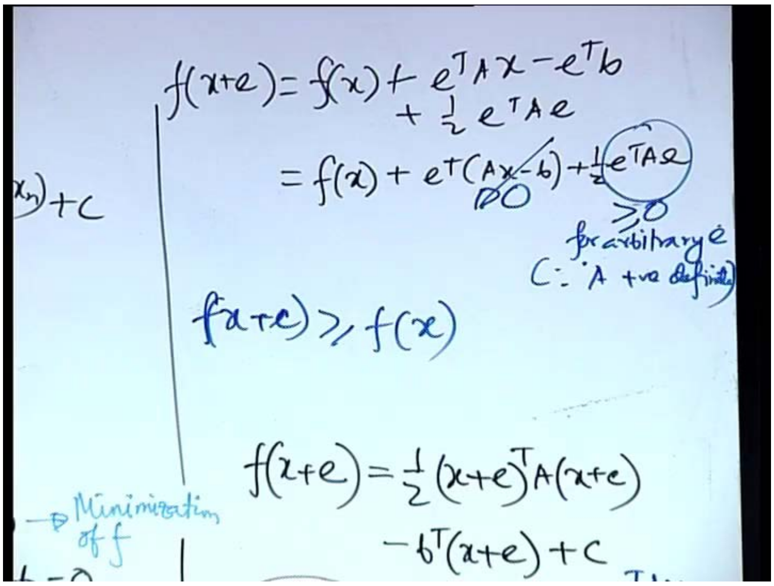

Now, if you combine all this terms, we can write f (x plus e) equal to f (x plus e) transpose A x minus e transpose b plus half e transpose A e because A x equal to b so if you have this equal to 0. So, it becomes f (x) plus half e transpose A e, because A is positive definite e transpose A is greater than equal to 0 for any arbitrary e so this is greater than equal to 0 for arbitrary e, since A is positive definite. So from here, what follows is that f (x plus e) is greater than equal to f (x); that means, any other functional argument with which is different from x is greater than makes the function f greater than the function with arguments of x.

So, f (x) is a minimum and not a maximum. So, what we can summarize from this discussion? we can summarize that if we construct a function f as half x transpose A x minus b transpose x plus c, where A is a symmetric and positive definite coefficient matrix, then minimization of f corresponds to the solution of the system A x equal to b that is what we can summarize from this so based on this technique therefore, one way go for a solution of the system A x equal to b not in a direct way, but in an indirect way with an approach so as to minimize the function f by constructing the function f and then minimizing that, and because it tries to traverse in a direction of the gradient of f and said that to 0, it is called as a gradient such method because it is searching the direction of the gradient and setting it to 0 so as to get the solution of the system of algebraic equations.

Now, this gradient search method has different varieties we will not go into the details of the gradient search method in this particular course, but, what we will try to do is? we will try to consider one or two very basic types of gradient search method and with very simply illustrative, examples try to understand the concept that is there behind implementation of this method, and the first of that kind is known as the steepest descent method.

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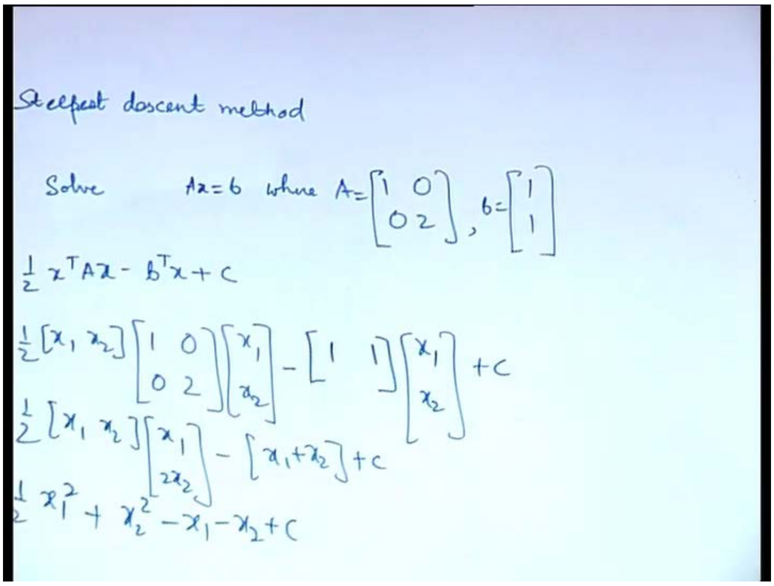

We will try to learn this method through a very simple example, let us say that we are interested to solve. Example, solve A x equal to b where A is equal to this 1 and b is equal to 1 1 so what we will do is we will first follow the step that we have identified through the initial prescription of the minimization problem, we have to first specify a minimization problem of a function. So, let us construct the function f, what is this, half x transpose A x minus b transpose x plus c so half x 1, x 2 minus 1 1 x 1, x 2 plus c so these becomes half of x 1 square plus x 2 square minus x 1 minus x 2 plus c. So, f represents a family of functions depending on the choice of c, so what does this family represent corresponding to f equal to 0.

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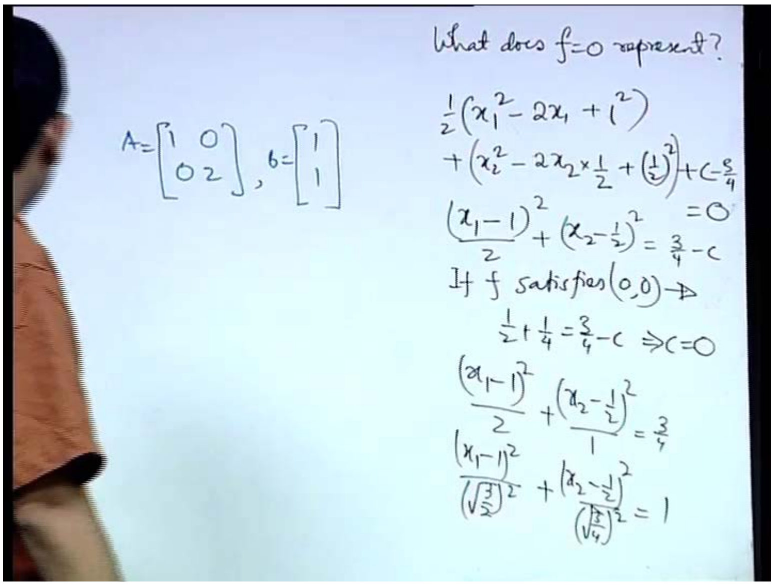

What does f is equal to 0 represent? So, let us do a bit of coordinate geometry for that, it is a two-dimensional situation, so we can interpret geometrically in a very simple way. So, we have half of x 1 square minus 2 into x 1 plus 2 square sorry 1 square plus x 2 square minus 2 into x 2 into half plus half square plus c, then what we have added extra? Half plus one-fourth that is three-fourth; so we subtract three- fourth that is equal to 0. So x 1 minus 1 whole square by 2 plus x 2 minus half whole square is equal to 3 by 4 minus c.

You can specify the choice of c by forcing this function to pass through a particular point. For example, if you allow it to pass it through 0 commas 0 so if f passes through or satisfies 0 comma 0, then half plus one-fourth is equal to three-fourth minus c. So, what is c? c is 0; remember choice of c is arbitrary. So, you can allow your function to satisfy a particular set of points and then find out the value of c accordingly. Next, what we will do is we will try to make a sketch of this function.

So the function is like x 1 minus 1 whole square by 2 plus x 2 minus half whole square by 1 is equal to three-fourth so, x 1 minus 1 whole square if you can multiply both the sides by 4 by 3 so here it becomes 2 into 3 by 4 so3 by 2 plus x 2 minus half whole square by 3 by 4 is equal to 1 so what does it represent? It represents an ellipse in the x 1, x 2 plane so, root over 3 by 2 whole squares then root over 3 by 4 whole squares sox 1 minus a x 1 minus alpha whole square by A square, plus x 2 minus beta whole square by b square equal to 1, where alpha is 1, beta is half, A is root 3 by 2 and b is root 3 by 4. So, what is the center of the ellipse one comma half.

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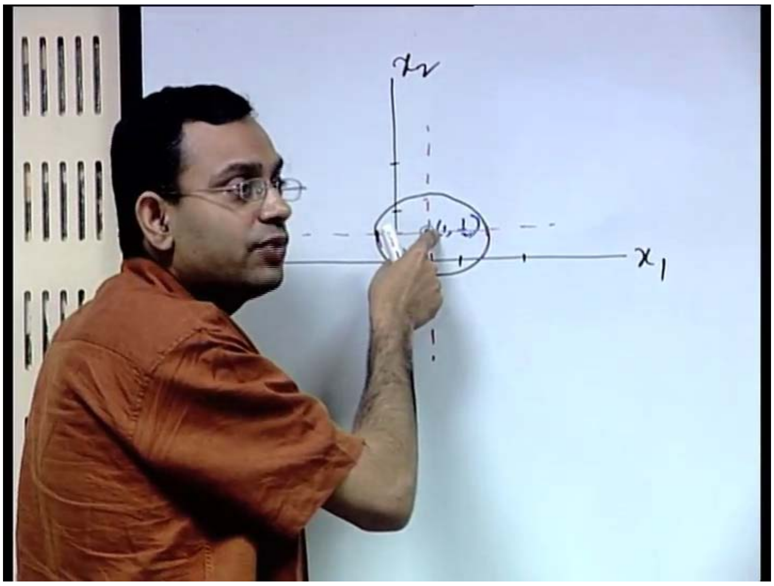

So, let us try to make the sketch as accurately as possible of course, rough sketch so, x 1 equal to 1, and x 2 equal to half so, 1 comma half. So, the major axis will be laid out along this direction minor axis will be laid out along this particular direction. So, x 1 minus 1 by root 3 by 2, so s A is root 3 by 2 so may be some distance like this, so, if we make a sketch of the function, I am just making the sketch arbitrarily, but it should be consistence it passes through 0 0, that is, how we are constructed the function f.

So, let us make a plan by looking into the geometrical form of these function, see this is a very simple system by looking into the equation you can see that it is x 1 equal to 1 and x 2 equal to half that is a solution. I have purposefully chosen this very simple system, because it will illustrate as something important, what it will illustrate, one comma half is the solution that we have seen from the system. Let us say that we start with an initial guess point as 0 commas 0 so we start with this point and we intend to hit this bulls eye when we start with this point and we intend to hit this bulls eye we will not be able to do it one short, because starting from this point, what is the direction in which you will be moving? Will be moving in the direction of gradient of f, that is the maximum rate of change of f till it comes to the minimum. So, the gradient of f, when we consider at this point, what it will represent? It will represent the normal direction to the curve, but normal direction to the curve is not going to the point to the center because this is not a circle, if it was a circle, it would have directly pointed towards the center because it is not a circle it will not directly point towards the center.

So, what it will do? It will point towards some direction which is not exactly this one so we will move in the in certain direction and the direction is what the direction is something very special, why it is special? Gradient of f is what; it is A x minus b that is what we have already found out so that is nothing but equal to minus r, where r is the residual so it has also something to do with the residual we have define the residual as b minus A x so we are moving along the direction of the residual at a particular point we move by certain distance and then we will stop and change the direction, because eventually we have to reach here so where to stop and change the direction and take a new direction in a way with an effort to reach here, is the next objective for us to learn and that we will take up in the next class. Thank you.